Understanding Scaling Relations In Fracture and Mechanical Deformation of Single Crystal and Polycrystalline Silicon By Performing Atomistic Simulations at Mesoscale

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  - -Limitations of MD simulations
- **Method and Framework**
  - - Equivalent crystal lattice method
- **Silicon nanowires/ polycrystalline silicon Results**
- **Conclusion and Future works**

Limitations of MD simulation

- **Discrepancy between MD simulation and experimental results**

1. **Length Scale**

   - Recent billion atoms simulation (1 x 1 x 1 μm for metal)
   - Most of MD simulation is nanometer scale (In many case, using only a small part of actual specimen for simulations)

2. **Time scale**

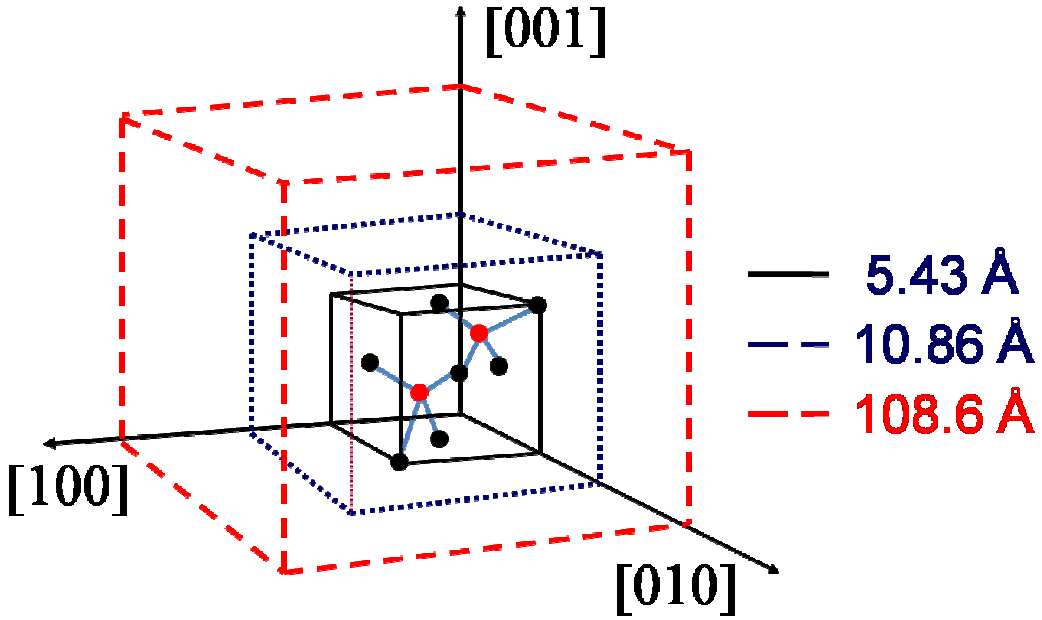
   - Most MD simulation's time step is femto second
   - Current time step extending methods can increase time step about factor of 15

- **Necessity to increase length and time scale of MD simulations**

Method and framework

- **Equivalent crystal lattice method**
- **New inter-atomic potential parameters**
  - Tersoff potential (T3)
- **Comparison of properties**
  - C11, C12, C44, Bulk modulus, Total lattice energy.
- **Time step calculations**
  - Maxwell-Boltzman distrubution
- **Simulation details**
  - Construction of suprtcells, NST ensemble,

Equivalent crystal lattice method



- Lattice parameters: 5.43, 10.86, 108.6, and 1086 Å

-Number of atoms in the unit cell are the same

--Fraction coordinates in the unit cell are the same

-Potential parameters are found by minimizing *F*

$$F = \sum_{i=1}^{N_{obs}} w_i (f_i^{tar} - f_i^{calc})^2$$

N_{obs} is the number of observables, f^{tar} and f^{calc} are the target and calculated values of the observables, and w_i is the weight factor for the given observables

Parameters for Tersoff potentials

Lattice Constant	5.43Å (T3)	10.86Å	108.6Å	1086Å
A (eV)	1830.8	9911.8	9682272.8	12256245358.6
B (eV)	471.18	2500	2500000.0	2846954605.4
λ_1 (Å^{-1})	2.4799	1.2125	0.1195	0.01235
λ_2 (Å^{-1})	1.7322	0.8166	0.08071	0.008282
α	0	0	0	0
n	0.78734	0.78734	0.78734	0.78734
β	1.0999E-06	1.0999E-06	1.0999E-06	1.0999E-06
n	0.78734	0.78734	0.78734	0.78734
c	100390	100390	100390	100390
d	16.218	16.218	16.218	16.218
h	-0.59826	-0.59826	-0.59826	-0.59826

$$E=\sum_i E_i=\tfrac{1}{2}\sum_{i\neq j} V_{ij}\ ,$$

$$V_{ij}=f_C(r_{ij})[a_{ij}f_R(r_{ij})+b_{ij}f_A(r_{ij})]$$

$$f_R(r)=A\ \exp(-\lambda_1 r)\ ,$$

$$f_A(r)=-B\ \exp(-\lambda_2 r)\ ,$$

$$f_C(r)=\begin{cases}1, & r<R-D\\ \tfrac{1}{2}-\tfrac{1}{2}\sin\left[\dfrac{\pi}{2}(r-R)/D\right], & R-D<r<R+D\\ 0, & r>R+D\end{cases} \qquad (1c)$$

$$b_{ij}=(1+\beta^n\zeta_{ij}^n)^{-1/2n}\ ,$$

$$\zeta_{ij}=\sum_{k\ (\neq i,j)} f_C(r_{ik})g(\theta_{ijk})\exp[\lambda_3^3(r_{ij}-r_{ik})^3]\ , \qquad (1d)$$

$$g(\theta)=1+c^2/d^2-c^2/[d^2+(h-\cos\theta)^2]\ ,$$

$$a_{ij}=(1+\alpha^n\eta_{ij}^n)^{-1/2n}\ ,$$

$$\eta_{ij}=\sum_{k\ (\neq i,j)} f_C(r_{ik})\exp[\lambda_3^3(r_{ij}-r_{ik})^3]\ . \qquad (1e)$$

Results comparison

Properties	Target values (experimental)	Tersoff (T3)	New potential		
		Lattice parameters(Å)			
		5.43 Å	10.86 Å	108.6 Å	1086 Å
C_{11} (GPa)	165.7	142.5 (14)	137.0 (17)	134.86 (18.6)	136.6 (17.5)
C_{12} (GPa)	63.9	75.4 (18)	70.0 (9.7)	68.13 (6.63)	73.5 (15)
C_{44} (GPa)	79.6	69 (13.3)	67.42 (15)	67 (15.8)	64.8 (18.6)
B (GPa)	98	98 (0.0)	98.5 (0.6)	90.37(7.7)	94.5 (3.5)
Lattice E (ev)	-37.36 (5.43Å) -298.88 (10.86Å) -298880 (108.6Å) -298880000 (1086Å)	-37.04(0.9)	-289.4 (0.14)	298387 (0.1)	-298935530(0.05)
Atomic mass	28.0855	28.0855	224.684	224684	224684000

Silicon nanowires Simulation detail

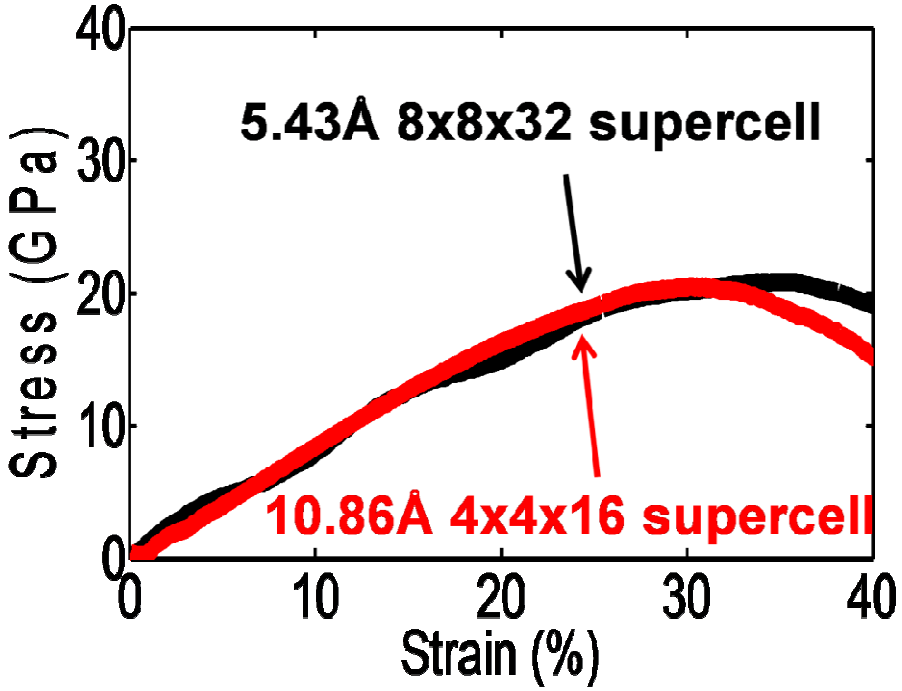
Supercell size	5.43 Å	10.86 Å	108.6 Å	1086 Å
4x4x32	2.17x2.17x17.36 nm (4096)	4.34x4.34x34.8 nm (4096)	43x43x348 nm (4096)	0.43x0.43x3.48µm (4096)
8x8x32	4.34x4.34x17.36 nm (16384)	8.7x8.7x34.8 nm (16384)	87x87x348 nm (16384)	0.87x0.87x3.48µm (16384)
16x16x32	8.7x8.7x17.36 nm (65536)	17.4x17.4x34.8 nm (65536)	174x174x348 nm (65536)	1.74x1.74x3.48µm (65536)

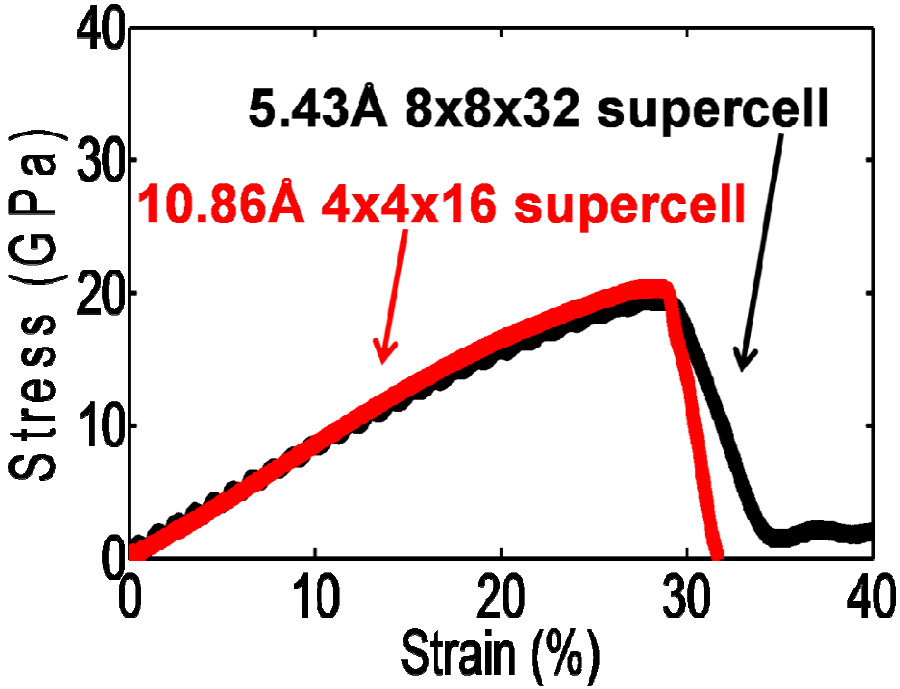
- **Applying tensile load constant strain rates: 0.01%/step and 0.001%/step**

- **NST ensemble (Constant particles, temperature, stress)**

- **Temperature : 300K, Nose-Hoover thermostat**

Simulation results between 5.43 and 10.86Å equivalent lattice

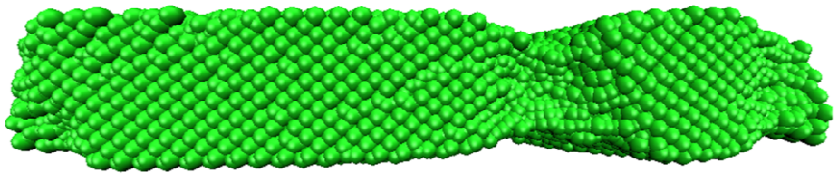




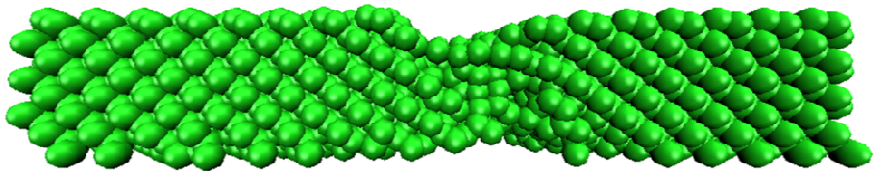
(a) strain rate 0.01%/step **(b) strain rate 0.001%/step**

Dimension: 4.34 x 4.34 x 17.36 nm

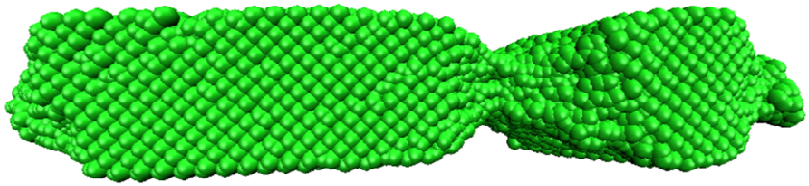
Fracture results between 5.43 and 10.86Å equivalent lattice



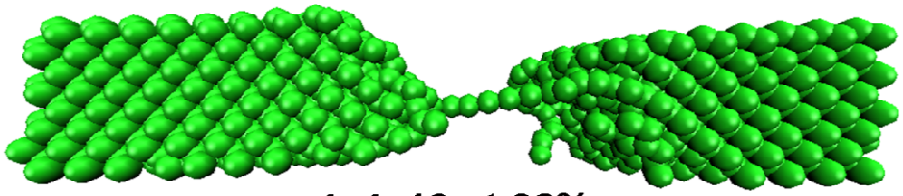
8x8x32 at 32%



4x4x16 at 30%



8x8x32 at 34%



4x4x16 at 32%

(a)

(b)

5.43 Å

10.86 Å

Dimension: 4.34 x 4.34 x 17.36 nm

strain rate 0.001%/step

Statistical analysis: Coefficient of correlation (R)

$$R = \sqrt{\frac{SSR}{SSTO}} = \sqrt{1 - \frac{SSE}{SSTO}}$$

$SSR = \sum (\hat{Y}_i - \bar{Y})^2$: Regression sum of square,

where $\bar{Y}$: mean value, $\hat{Y}_i$: value from the fitted line

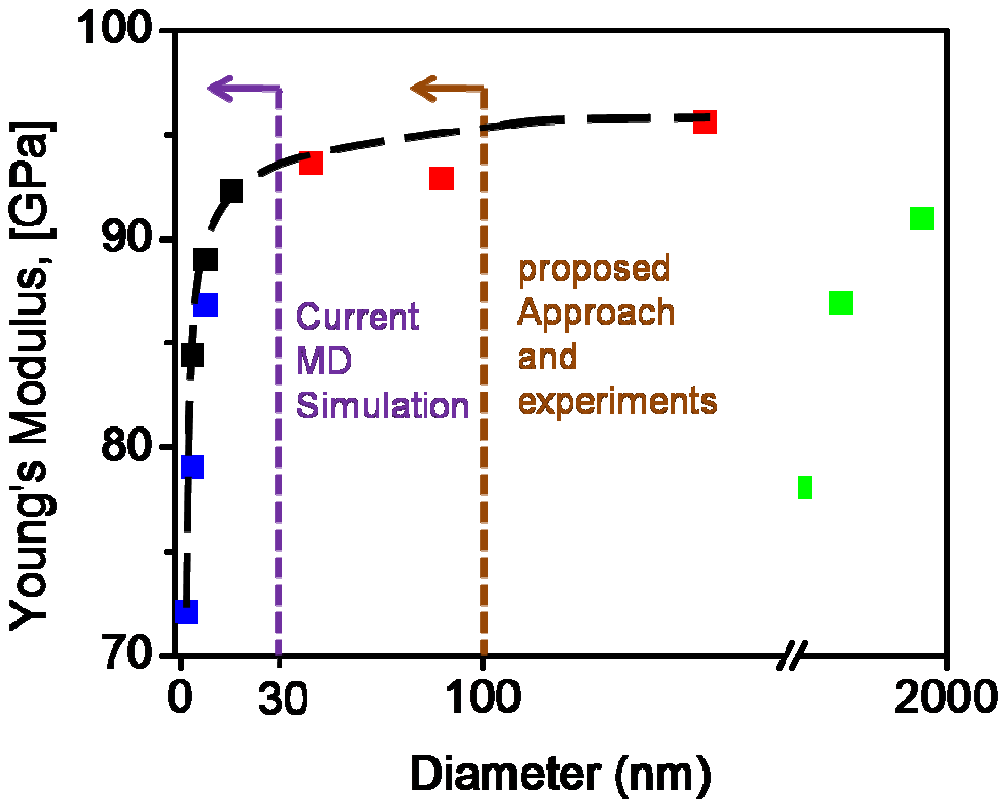
$SSE = \sum (Y_i - \hat{Y}_i)^2$: Error sum of square

$SSTO = SSE + SSR$: Total sum of square

Properties	Predictor variables			
	Diameter	Surface area	Volume	Surface to volume ratio
Young's modulus	0.14	0.10	0.15	-0.74
Fracture stress	0.30	0.25	0.26	-0.85

- The surface to volume ratio is most critical factor

Young's modulus transition diameter (Si nanowire)



Discrepancy b/w current MD and experiments

-Current MD predicts 4-30nm for transition diameter (Park et al., MRS bulletin, 34, 2009)

-Experiments measured100nm for transition diameter (Li et al. Appl.Phys.Lett, 83,2003 qnd Han et al. adv. Mater.,19, 2007)

-Our simulation predicted around 100nm for transition diameter

Polysilicon simulation detail (Number of atoms and sizes)

	5.43 Å	10.86 Å	108.6 Å	1086 Å
8 grains	49356 (101x101x101 Å)	49356 (202x202x202 Å)	49356 (2020x2020x2020 Å)	49356 (20200x20200x20200 Å)
64 grains	48058 (101x101x101 Å)	48058 (202x202x202 Å)	48058 (2020x2020x2020 Å)	48058 (20200x20200x20200 Å)

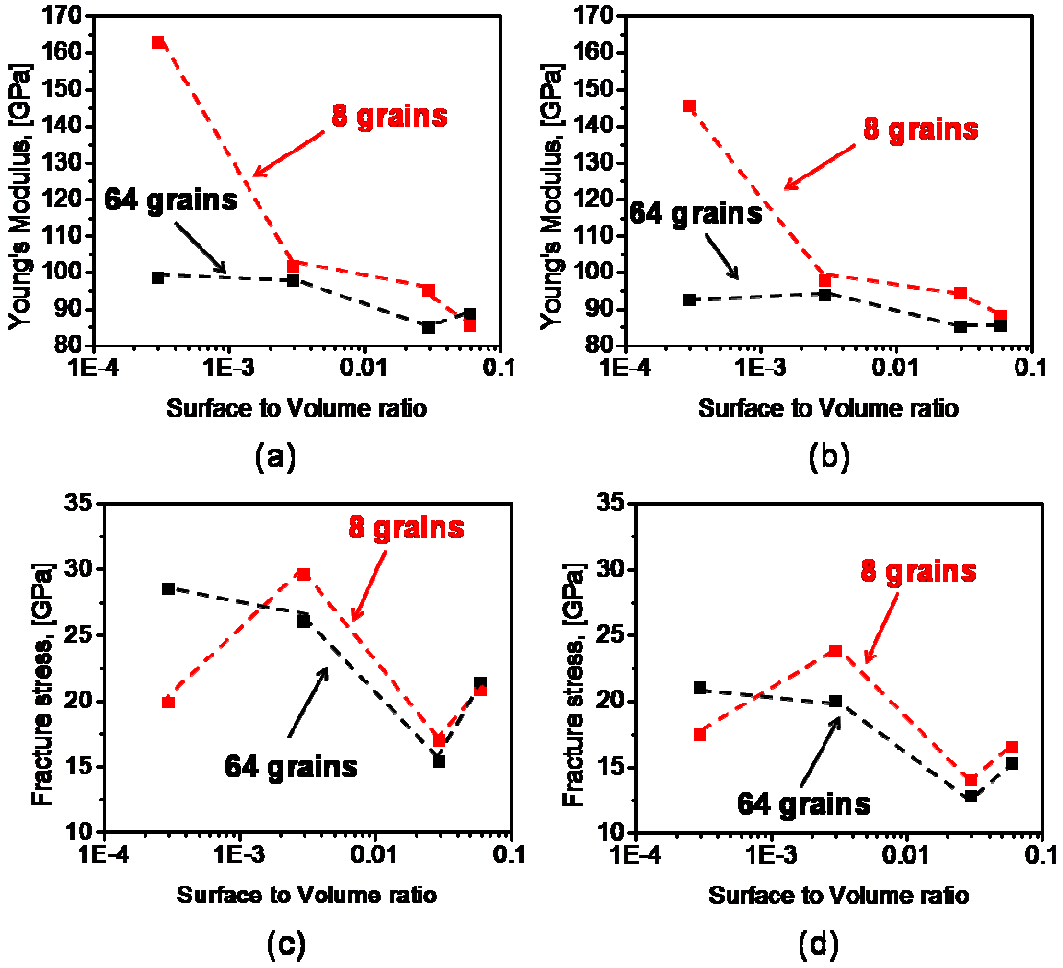
- **Constructed bulk polysilicon and surfaced polysilicon**

- **Applying tensile load with constant strain rates: 0.01%/step and 0.001%/step**

- **NST ensemble (Constant particles, temperature, stress)**

- **Temperature : 300K, Nose-Hoover thermostat**

Number of grain and surface effect on properties



(a)Young's modulus with strain rate 0.01%/step

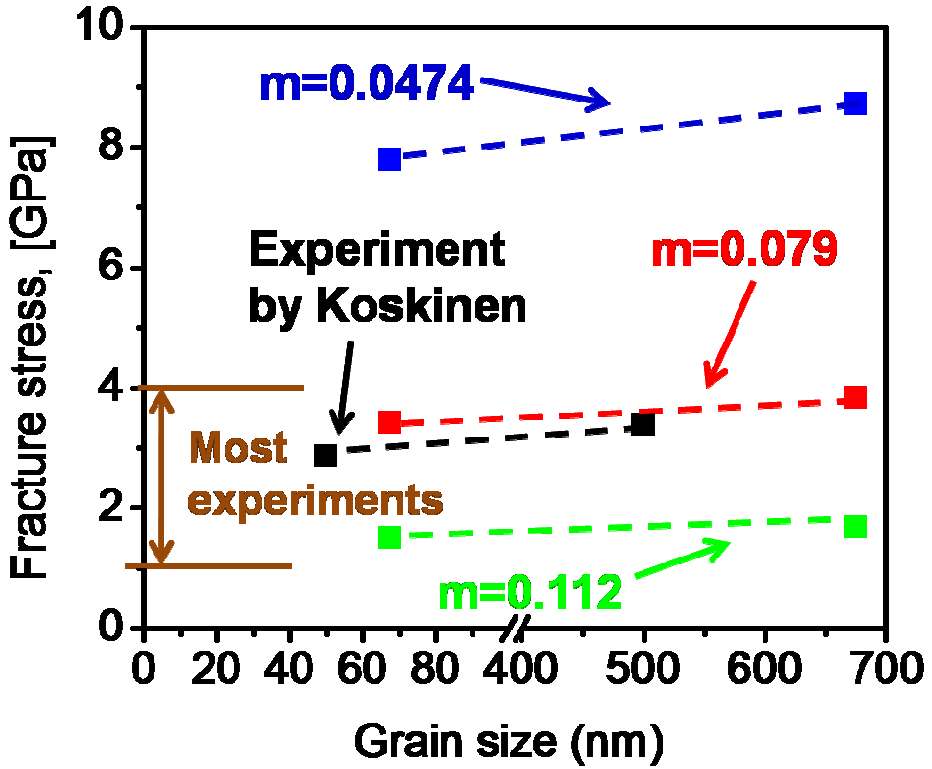
(b) Young's modulus with strain rate 0.001%/step

(c) fracture stress with strain rate 0.01%/step

(d) fracture stress with strain rate 0.001%/step

- With the same surface to volume ratio (same dimension), number of grain changes the Young's modulus: Grain size effect

Comparison with experiments



-Koskinen et al. measured fracture stress with various grain size

- Inverse Hall-Petch mechanism

- Our results agree with Koskinen's experiments

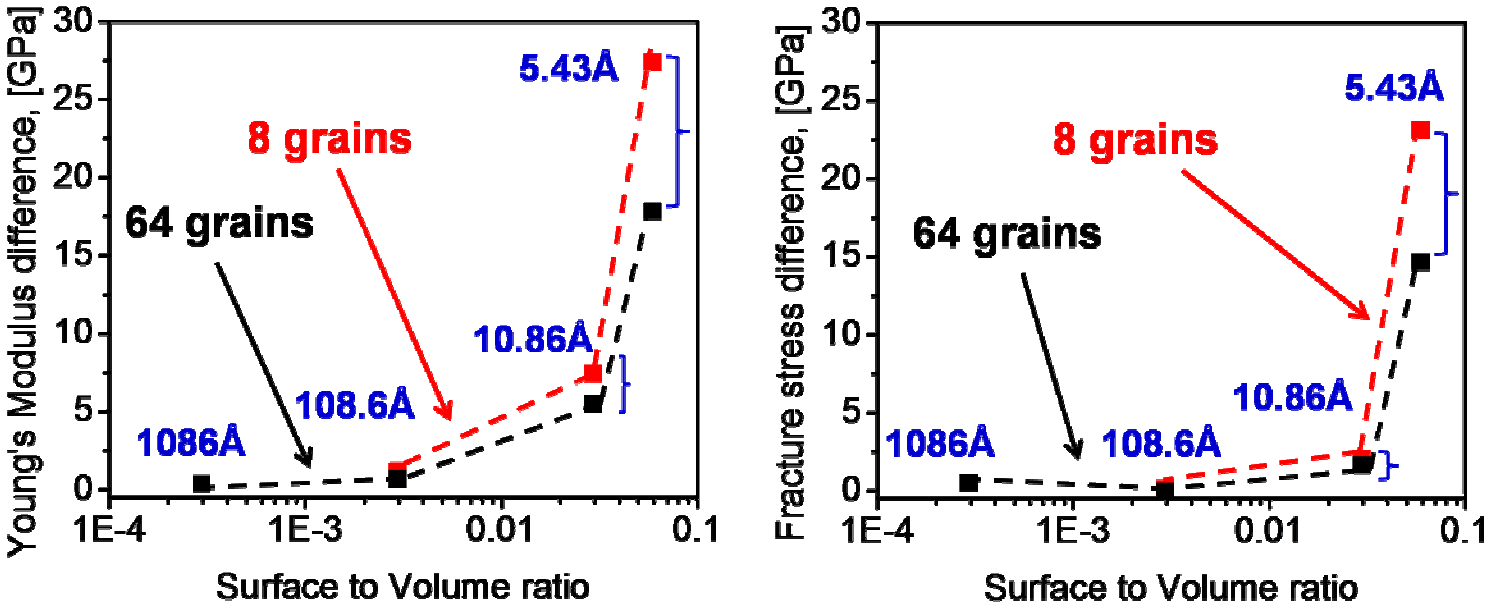
- Our fracture stresses are converted assuming typical experimental strain rate 2E-3/sec

$$\frac{\sigma}{\sigma_0} = \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right)^m$$

σ : stress, $\dot{\varepsilon}$: strain rate, m : strain rate sensitivity index

($0.0474 \le m \le 0.112$, avgerge $m = 0.079$)

Limit of surface and grain size effects on polysilicon



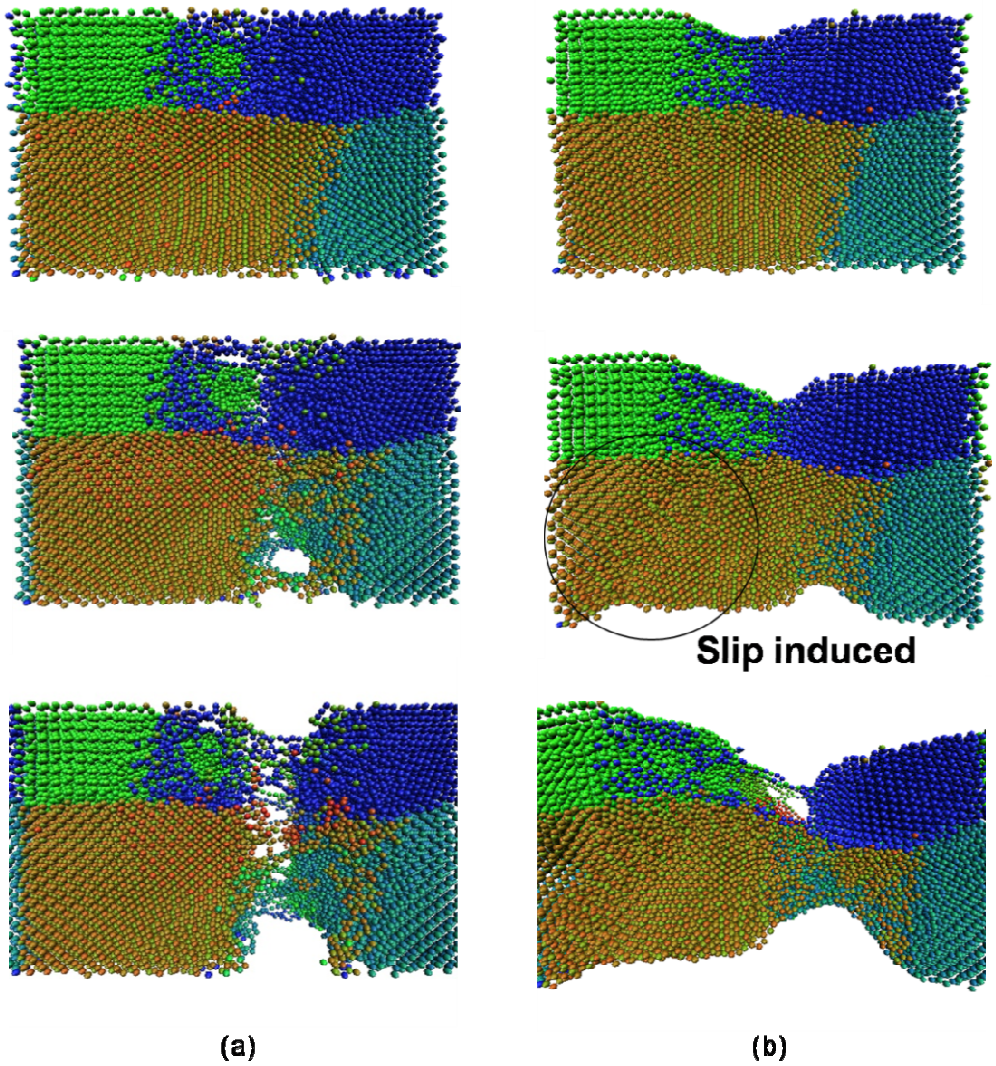
strain rate 0.01%/step

- Grain size effect and surface effect is decreasing and converge to 0 !!

- About 1 μm of the grain size and 2^3 μm^3 of specimen size are the limit above which the Young's modulus and fracture stress is not influenced by grain size as well as surface for polysilicon

  - Agree with experiments by Fancher et al. , J. Mater. Sci., 36, 2001,

Fracture transition from brittle to ductile with surfaces



(a) bulk polysilicon

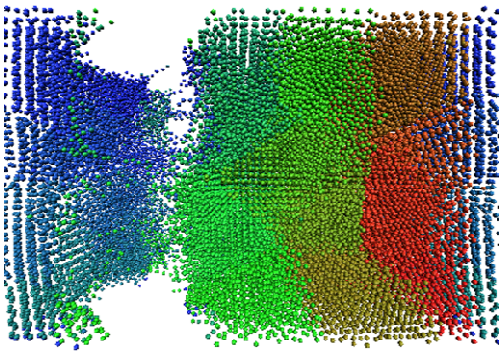
(b) surfaced polysilicon

101 x 101 x 101 Å 8 grain polysilicon with strain rate 0.001%/step

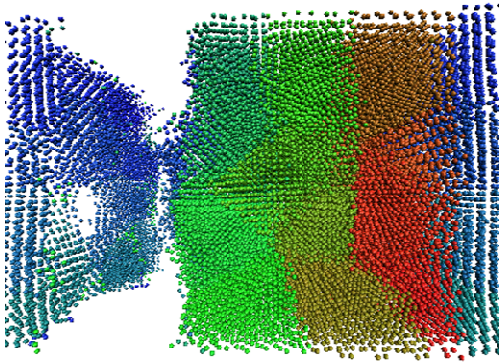
-Surfaces make materials more ductile when compared to bulk materials

-Slip induced fracture is observed inside grain

Fracture behaviors for equivalent lattices



(a)



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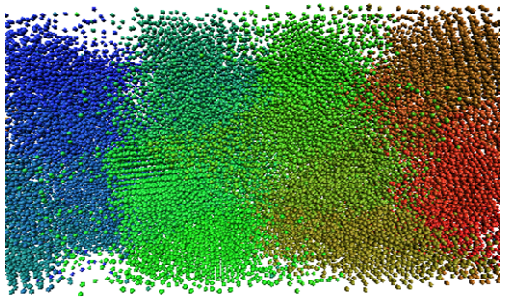
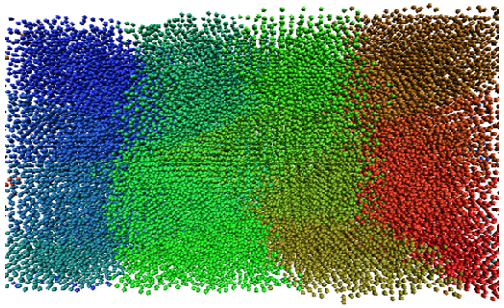


(c)



(d)

(a) 5.43 Å lattice
(b) 10.86 Å equivalent lattice
(c) 108.6 Å equivalent lattice
(d) 1086 Å equivalent lattice

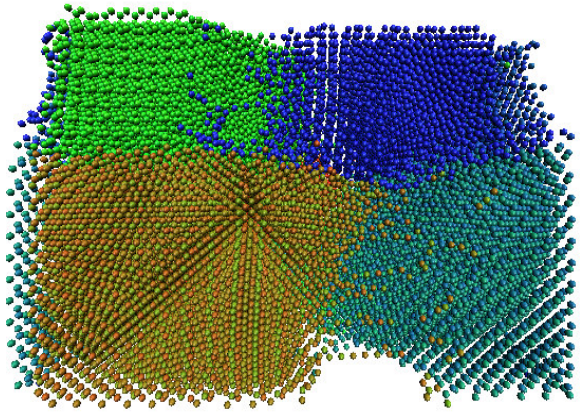
64 grain bulk polysilicon with strain rate 0.001%/step

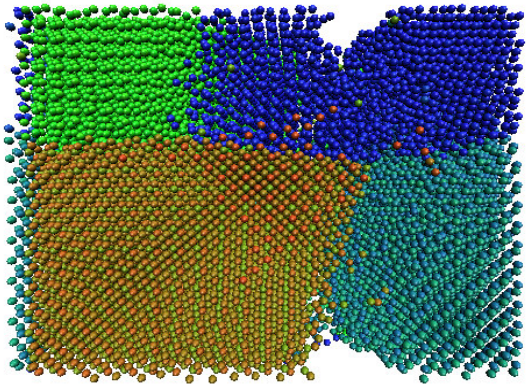
-Fracture initiation, propagation, final pattern are identical b/w 5.43 Åand 10.86 Å

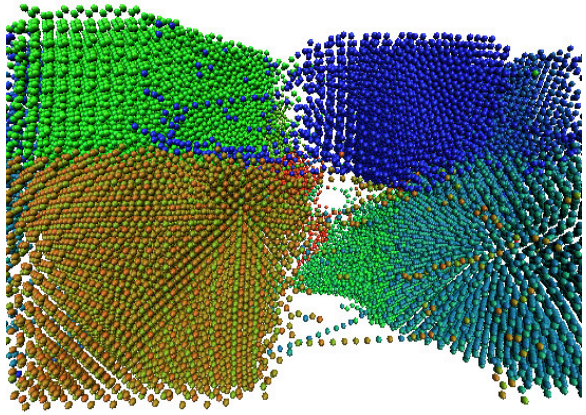
-Fracture initiations are identical for all lattices

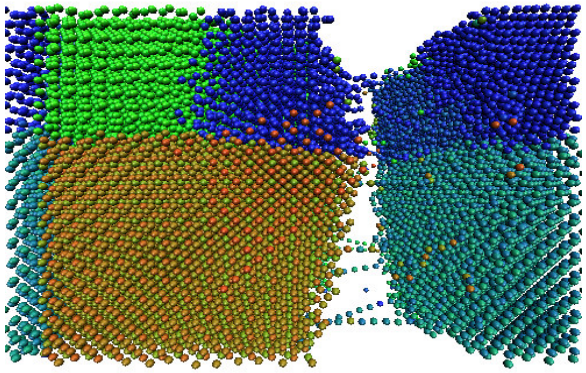
-Temperature s are higher than 300K for 108.6Å and 1086Å

Intergranula vs. transgranula depending on strain rate









(a) (b)

Sz2 gs1sr1 and sr2 - surface

202 x 202 x 202 Å 8 grain surfaced polysilicon with strain rate with 10.86Å equivalent lattice
(a) 0.01%/step (b) 0.001%/step

-Fracture propagation depends on strain rate

-Mostly, intergranula

-Transgranula observed

Conclusion

- **By using equivalent crystal lattice method,**
  - Time step increased about factor of 500 (From 0.001 to 0.5fs)
  - Length scale increased factor of 200 (5.43 Å to 1086 Å)

- **The surface to volume ratio is the most important factor at nanometer and micron scale**

- **MD simulation results are more close to experiments if actual specimen dimension is used for MD simulations**
  - Young's modulus transition diameter (Si nanowire)

Conclusion

- **MD simulations of polysilicon with grain sizes ranging from 3.4nm to 1.3 μm are made possible using equivalent lattices**

- **Inverse Hall-Petch mechanism is observed for polysilicon**
  - Agrees with experiments, opposite to metals and alloys

- **The Young's modulus is not influenced by grain size when grain size is larger than 7nm for bulk polysilicon**
  - Verified by DFT calculations

- **The Young modulus is strongly influenced by grain size for surfaced polysilicon**

- **The existence of surfaces make materials more ductile when compared to bulk materials**